LDRD FY 2015 RESOURCES REQUEST PLAN

1.0 APPROVAL RECORD

- Reviewed by: Document Control Coordinator (Amy Tehan)
- Approved by: Chief Operations Officer (Mark Murphy)
- Approved by: Associate Laboratory Director for Sponsored Research (Deb Covey)
- Approved by: Assistant Director for Scientific Planning (Cynthia Jenks)
- Approved by: Chief Research Officer (Duane Johnson)
- Approved by: Deputy Director (Tom Lograsso)
- Approved by: Director (Adam Schwartz)

The official approval record for this document is maintained in the Training & Records Management Office, 151 TASF.

2.0 REVISION/REVIEW INFORMATION

The revision description for this document is available from and maintained by the author.

3.0 PURPOSE AND SCOPE

This document acts as official request for Ames Laboratory's annual LDRD expenditures.

3.1. Definitions

- LDRD – Laboratory Directed Research and Development
- LDRD Key Components:
  - *Strategic Initiatives* – employee- initiated proposals that address at least one of the strategic goals or an area of potential growth within AMES' initiatives for the current fiscal year.
  - *Novel Projects* – a balance of basic, applied, single-investigator, and multidisciplinary projects in new areas or directions, not necessarily in direct support of our strategic initiatives.
  - *Exceptional Opportunities* – an integral part of the pursuit of capabilities in a strategic area that enhances human and physical resources to support that area. This component consist of projects that do not fit neatly into the other two components or that can arise outside the normal fiscal-year schedule, e.g., strategic hires, collaborations with external institutions where a superior expertise resides, or projects offering exceptional R&D opportunities for AMES.

4.0 PROGRAM/POLICY/PROCEDURE INFORMATION

In FY2015, the Ames Laboratory requests approval for an LDRD expenditure comprising 3% of AMES' projected FY total costs, **estimated to be approximately $1.3M**. The Director proposes a funding portfolio shown in **Tables 1 and 2** for the most recent, current, and next fiscal year, supporting the *Strategic Initiatives*, *Novel Projects, and Exceptional Opportunities.* These projects' datasheets are provided in addition to this Plan for DOE review and approval.

The Laboratory's request reflects management's best judgment as to the optimal balance between LDRD funds with their inherent flexibility and funds needed to accomplish programmatic deliverables for current sponsors while satisfying competing demands on Laboratory overhead. By insuring an adequate LDRD resource, laboratory management has a more effective tool to open new opportunities for creative Science & Technology directions and to adjust rapidly to new mission needs of the Department.

Due to the nature of exploratory research we cannot predict precisely to what program a given project may turn out to be most valuable over time. Nonetheless, the Congress of United States understands this role of exploratory R&D that underlies its granting the directors of national laboratories the opportunity to pursue laboratory-directed R&D and enables the laboratories to manage this vital resource and insuring its productivity and relevance to the needs of the Nation.

4.1. LDRD Reporting

Annual LDRD program plan (this resource request plan) is required at the Ames' Site Office at least 45 days before the start of the fiscal year. In addition, LDRD Portfolio Tables will be provided in 4.2.

In addition, a *summary report* from each principal investigator must be prepared for a brief annual report on their project within sixty days of the end of the fiscal year. An Office WORD Document Template prepared by LDRD Program is available from program office and website. The LDRD Program Coordinator compiles these individual reports and prepares an Annual Report on the LDRD program for submission, which is required within 6 months after the end of the fiscal year. The CRO, LDRD Program Administrator, and Budget will work together on Budget and Reporting to Site Office and DOE.

As required in Reporting Requirements (Section 7, LDRD Plan 30000.001), a "datasheet" template is required from each principal investigator during the pre-approval process, so as to provide project summary information (Title, Brief Abstract, Lead Investigators, and Estimated Cost). Summary information from these datasheets goes to the Ames' Site Office, which will make them available to appropriate entities, including Congress. Datasheets must be submitted to Site Office at least 30 days prior to the start of the fiscal year to allow at least 30 days for review; for late-start projects, datasheets may be submitted any time in the fiscal year.

4.2. LDRD Portfolio Tables

The Director proposes a funding portfolio shown in **Tables 1(A and B) and 2** for the most recent, current, and next fiscal year.

TABLE 1.A FY 2013 INVESTMENT AREAS (Actual)

	Distribution of LDRD Investment ($ K)	Planned Distribution of Investment ($ K)
Novel Projects		**$180**
[projects] *FY13-14: Dynamic Whitelist Generation for Automated Intrusion Response* *FY13-14: Femtosecond-resolved polarimetry probes of electronic nematicity in iron-pnictides*	$89 $49	
Novel Projects Subtotal	$138	**$180**
Exceptional Opportunities *(includes Spedding Post-doctoral Fellowships)*		**$360**
[none]*	$0*	
Exceptional Opportunity Subtotal	$0*	**$360**
Strategic Initiative Areas		**$360**
Materials Discovery, Design, Development (MaDDD) Science		$90
FY13-14: Demystifying the hydration layer on nano-oxides in suspensions by liquid cell transmission electron microscopy	$68	
Greener Advances in Catalysis and Energy (GrACE) Formerly: Catalyzing a Greener Future		$180
FY13-14: Atomic and electronic level control of nanocluster catalysts encapsulated in metal-organic frameworks *FY13: In-situ, real-time imaging of single-site catalysts under turnover conditions*	$102 $102	
Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE). Formerly: Center for Solid-state NMR Science		$45
[none]	$0	
CREEM – Center for Rare-Earth and Energy-critical Materials **(graduated initiative, ends 30 Sept 2013)**		$45
FY13-14: *Rapid, small-scale, high-purity, rare-earth metal preparation*	$63	
Strategic Initiative Subtotal	$335	**$360**
Subtotal	$473	
LDRD Administration Overhead	$35	
Total FY 2013 LDRD Program	$508	$900 (approved)

*Exceptional opportunity hire was expected but started nearer end of FY13.

TABLE 1.B FY 2014 INVESTMENTS (Actual, as of 1 August 2014)

	Distribution of LDRD Investment ($K)	Planned Distribution of Investment ($K)
Novel Projects		**$270**
FY13-14: *Dynamic Whitelist Generation for Automated Intrusion Response*	$232	
FY13-14: *Femto-second-resolved polarimetry probes of electronic nematicity in iron-pnictides*	$41	
Novel Projects Subtotal	$273	**$270**
Exceptional Opportunities *(includes Spedding Post-doctoral Fellowships)*		**$130**
None awarded	$0	
Exceptional Opportunity Subtotal	$0	**$130**
Strategic Initiative Areas		**$700**
Materials Discovery, Design, Devel. (MaDDD) Science		$300
FY13-14: *Rapid, small-scale, high-purity, RE metal prep.*	$45	
FY13-14: *Demystifying the hydration layer on nano-oxides in suspensions by liquid cell TEM*	$135	
FY14-15: *Self-healing, adaptive structural coatings*	$70	
FY14-15: *Adsorption-induced, Shape-changes in Nanoalloys: extended Wulff construction with first-principles calculations*	$55	
Greener Advances in Catalysis and Energy (GrACE)		$220
FY13-14: *Atomic and electronic level control of nanocluster catalysts encapsulated in metal-organic frameworks*	$105	
FY14-15: Customized Assembly of Catalytic Systems by 3D Printing Technology	$144	
SS-NMR: Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE).		$180
FY14-16: *Sensitizers for DNP-NMR Spectroscopy*	$172	
Strategic Initiative Subtotal	$726	$700
Subtotal	$999	$1,100
LDRD Administration Cost (estimated to EOY)	$104	$100
Total FY 2014 LDRD Program	$1,103	$1,200 (approved)

TABLE 1.C FY 2015 INVESTMENTS (continuations, not all down-selects, as of 1 August 2014)

	Distribution of LDRD Investment ($K)	Planned Distribution of Investment ($K)
Novel Projects		**$200**
FY13-14: Dynamic Whitelist Generation for Automated Intrusion Response (FY15 3rd-yr request under review)	$TBA	
FY15 Down-selected TBA	$TBA	
Novel Projects Subtotal	$TBA	**$200**
Exceptional Opportunities *(includes Spedding Post-doctoral Fellowships)*		**$140**
FY15-17: *Spedding Fellowship* (Study of Novel Materials using DNP-NMR Spectroscopy)	$138	
Exceptional Opportunity Subtotal	$138	**$140**
Strategic Initiative Areas		**$860**
Materials Discovery, Design, Development (MaDD)		$420
FY14-15: Self-healing, adaptive structural coatings	$72	
FY14-15: Adsorption-induced, Shape-changes in Nanoalloys: extended Wulff construction with first-principles calculations	$57	
FY15 Down-selected TBA	$TBA	
Greener Advances in Catalysis and Energy (GrACE)		$240
FY14-15: Customized Assembly of Catalytic Systems by 3D Printing Technology	$118	
FY15 Down-selected TBA	$TBA	
SS-NMR: Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE)		$200
FY14-16: Sensitizers for DNP-NMR Spectroscopy	$175	
FY15 Down-selected TBA	$TBA	
Strategic Initiative Subtotal	$TBA	$700
Subtotal	$1,200 (est.)	$1,200
LDRD Administration Cost (estimated to EOY)	$100 (est.)	**$100**
Total FY 2015 LDRD Program	$1,300	$1,300 (approved)

TABLE 2.A LDRD PORTFOLIO INVESTMENT

FY2013 is the first year of approved LDRD funding, as reflected in Table 1 above.
FY2014 totals as reflect in Table 1 above (starts as of 12/15/13).
FY2015 are projected.

LDRD COMPONENTS	FY2013 (%) Actual	FY2014 (%) Actual	FY2015 (%) Projected	FY2016 (%) Projected
Novel Projects	15.3%	23%	15%	15%
Exceptional Opportunities [Projects] and *Spedding PD Fellowships*	0%*	0%	11%	17%
Investments in Strategic Initiatives	37.3%	60.5%	66%	60%
Materials Discovery, Design, Development (MaDDD) Science	7.6%	25.4%	32%	30%
Greener Advances in Catalysis and Energy (GrACE) Formerly: Catalyzing a Greener Future	22.7%	21.0%	19%	15%
Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE). Formerly: Center for Solid-state NMR Science	0%	14.1%	15%	15%
CREEM – Center for Rare-Earth and Energy-critical Materials **(ended 2013)**	7%	n/a	n/a	n/a
LDRD Administrative Cost	3.9%	8.7%	8%	8%
USED % LDRD	56.5*	92.3%	100%	100%
UNUSED % LDRD	43.5*	6.7%	0%	0%

ADDITIONAL INFORMATION

FY2015 Strategic Initiative Area and Summaries

A-1: Materials Discovery, Design, and Development (MaDDD) Science

We will continue to expand a broader set of integrated capabilities for effective and efficient search methodologies for new energy-critical materials, including structure and chemistry prediction, with new functionalities.

Both theory and experiment are needed to inform the synthesis process and must be developed in parallel and integrated into the materials discovery. The new ideas and techniques will be coordinated with large-scale, predictive computational methods and new synthesis, processing and characterization to yield novel, valid design materials.

This LDRD thrust brings to be bear advanced simulation, modeling and theory, as well as advanced in situ probes and characterization techniques.

GOALS for FY13-15 LDRD – To enhance existing methods or to develop novel approaches (both theory and experiment), so as to inform the synthesis and processing needed for new energy-critical materials with new functionalities, or characterization of unique materials.

Focus Areas for Potential Funding (not exhaustive)

1. Computational materials discovery and design with experiment, especially involving integrated and rapid feedback for materials synthesis and processing of materials.
2. Optimization and selection tools, and algorithm development, e.g. for structural transformation pathways, for ground-state prediction; Database and/or Data Discovery techniques for materials.
3. Synthesis and Processing, including new synthesis optimization protocols
4. Novel or improved characterization tools.
5. Applied math/software engineering to enhance materials discovery, e.g., autotuning; adaptive programming; multi-level parallelism; software to reduce energy usage by computers.

A-2: Greener Advances in Catalysis and Energy (GrACE)

Catalysis is a critical component in US manufacturing, from fuel production to chemical synthesis for technologies and everyday products. In particular, new catalytic materials are imperative to the development of a green economy, including industrial catalysts and specially designed catalysts for biomass conversion that provide less waste, promote carbon sequestration, and reduce our dependence on foreign energy sources.

The AMES core capabilities in chemical and molecular sciences provide the necessary foundations for this initiative in experimental and computational design, synthesis and analysis of catalysts.

GOALS for FY13-15 LDRD – Continue to develop our leadership in predictive catalysis for a cleaner environment and more energy-efficient process streams, particularly using cooperative and 3D multifunctional catalysts. We will also find alternatives to rare earth containing catalysts in partnership and leveraging capabilities in CREEM and related efforts, such as Critical Materials Institute (CMI).

Focus Areas for Potential Funding (not exhaustive)
1. Electrocatalysis
2. Biomimetic Catalysis
3. Computational Tools for Catalysis Design
4. Development of capabilities through external partnering (e.g., with Argonne M2M effort).

A-3: Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE): our Solid-State NMR initiative

The Ames Laboratory has a unique concentration of solid-state NMR expertise, with several PIs being recognized as “undisputed world-wide leaders in the field”. Towards our goals of establishing a center focused on solid-state nuclear magnetic resonance (NMR) science, we will address scientific drivers relevant to the mission of DOE, including:

- Provide DOE with a leadership position in enhanced solid-state NMR characterization methods, especially Dynamical Nuclear Polarization (DNP) NMR.
- Move the frontiers of solid-state NMR techniques in several areas, e.g., improved characterization of catalytic, complex biomolecular and inorganic materials.
- Take advantage of our unique concentration of solid-state NMR expertise.
- Enable others to access the AMES expertise in solid-state NMR characterization.

GOALS for FY13-15 LDRD – We will provide leadership positions with new world-class NMR capabilities to enable the design and discovery of new materials.

Focus Areas for Potential Funding (not exhaustive)

1. Dynamic nuclear polarization (DNP) SS-NMR development
2. Novel methods for analysis of catalysts and biomolecular materials